Reevaluating the Hartman Effect for Field Emission

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(Dated: October 19, 2021)

An electron wave packet tunneling through a barrier has a transmission (or “group delay”) time τ_g that, for a rectangular barrier, is commonly held to become independent of the barrier width L as the width increases (the *McColl-Hartman effect*). In the present study, it is shown that: first, the McColl-Hartman effect for a rectangular barrier is dependent upon L as the Gamow tunneling factor $\theta(k)$ vanishes, and τ_g is only independent of L when $\theta(k)$ is large; and second, for a triangular barrier to model field emission, although τ_g can be large for small field, it vanishes when the energy matches the barrier height.

The question of how long an electron spends tunneling through a barrier has taken on increasing importance for nanogap devices [1–6] such as nanoantennas for which field emission occurs across an anode-cathode (AK) gap of 50 nm [7] down to 8 nm [8] (where the anode-cathode transit time [9] is on the order of femtoseconds), and attosecond experiments [10–12]. In his consequential study of tunneling across thin insulating layers using a model for which an incident wave packet encounters a rectangular barrier, Hartman [13] and earlier, McColl [14] found that the transmission time for a metal-insulator-metal (MIM) thin film was given by the group delay $\tau_g = \hbar/\sqrt{\mu\Phi}$ in the limit of large barrier width, where μ is the Fermi level and Φ is the vacuum work function: for a generic case where $\mu = \Phi = 1$ eV, then $\tau_g = 0.65821$ fs and, parenthetically, is smaller than but comparable to the barrier width-dependent semiclassical time of Büttiker and Landauer [15] of $\tau_{sc} = L/\sqrt{2\Phi/m} = 1.6860$ fs for $L = 1$ nm, but of a very different nature as demonstrated by Winful [16, 17], who demonstrated that τ_g was the sum of a dwell τ_d and self-interference τ_i time.

Our study of wave packet interactions with barriers using a time dependent Wigner distribution function (WDF) approach [18] indicate that rectangular barriers (and others with similar abrupt transition behavior) have properties that make their usage for wave packets problematic for simulations, even though plane wave and exponentially growing/decaying solutions are highly advantageous. Specifically, wave packets of finite momentum spread contain $k > k_v$ contributions, where $\hbar^2 k_v^2/2m = V_o = \mu + \Phi$ is the barrier height. In the $L\kappa \gg 1$ limit where $\kappa = \sqrt{k^2 - k_v^2}$, the sine functions

in the transmission probability $D_{rec}(k)$ becomes highly oscillatory and possesses numerous peaks ($D(k_n) = 1$) where $L\sqrt{k_n^2 - k_v^2} = \pi n$ for n integer [19]. This is in sharp contrast to the step barrier for which $D_{step}(k) = 4k\kappa/(k + \kappa)^2$ asymptotically approaches unity. A model that smoothly and asymptotically approaches the step limit is preferable for modeling field emission. The present study provides it in the following steps. First, as per Winful, attention is explicitly restricted to energy eigenstates $\psi_k(x)$ (not wave packets). Second, the analysis of Winful is recast using the Gamow factor $\theta(k)$ to allow generalization. Third, the Gamow analysis is repeated for a barrier characteristic of high field electron emission. Several candidates are available: (i) the image charge or Schottky-Nordheim (SN) barrier [20]: it describes field emission from metals [21] and semiconductors [22] and has a semi-analytic Gamow factor $\theta(k)$, but the transmission $t(k)$ and reflection $r(k)$ coefficients must be calculated numerically; (ii) the Eckart barrier [23]: it is an asymmetric barrier for which $t(k)$ and $r(k)$ are analytic, but the Gamow factor $\theta(k)$ must be calculated numerically; and (iii) the triangular or Fowler-Nordheim (FN) barrier [21] for field emission: it neglects image charge effects but $t(k)$, $r(k)$, and $\theta(k)$ are all completely analytic. Therefore, only the triangular barrier of choice (iii) is a simple and purely analytic representation of field emission under high field conditions (and is the most iconic example of tunneling wave mechanics [24, 25]). The consideration of the choices (i) and (ii) shall be taken up in a separate study [26] (but see the description given in the *Supplementary Material*). Thus, the FN formalism [27–29] is used for development and

analysis of the dwell τ_d and self-interference τ_i times.

The much discussed independence of τ_g on the width L of the rectangular barrier as L increases is termed the ‘‘Hartman effect’’: the dependence had been anticipated separately by McColl, so that the designation ‘‘McColl-Hartman’’ is preferable [30] and used herein. Hartman’s description (the ‘‘transmission time’’ τ_g becomes ‘‘independent of barrier thickness and small compared to the ‘equal time’ ’’, where ‘‘equal time’’ is the time required for a free incident packet to cover a distance L) is expressed equivalently by others as: ‘‘(t)he Hartman effect is the saturation of the group delay with barrier length’’ (Winful [16]); ‘‘Hartman observed that the transmission time approaches a constant for most energies less than the barrier height (except for energies *very close to the barrier height* or very close to zero)’’ (emphasis added, Smith and Blaylock [31]); ‘‘...a simple phase time following the calculation of Hartman... turns out to be independent of the thickness a of the barriers...’’ (Petrillo and Olkhovsky [32]); and ‘‘the time taken to traverse a barrier appears to be independent of the length of the barrier when said barrier is sufficiently broad.’’ (Rivlin, *et al.* [30]). The rectangular barrier is given by

$$V_{rec}(x) = V_o \Theta(x) \Theta(L - x) \equiv \frac{\hbar^2 k_v^2}{2m} \Theta(x) \Theta(L - x) \quad (1)$$

where $\Theta(x)$ is the Heaviside step function, $V_o = \mu + \Phi \equiv \hbar^2 k_v^2 / 2m$ is the barrier height, and L is the barrier width. Winful [16, 17] demonstrates that τ_g is the sum of a dwell time τ_d and a self-interference time τ_i , respectively, given as (compare τ_d to Eq. (2) of Ref. [15])

$$\tau_d(k) \equiv \left(\frac{m}{\hbar k} \right) \int_0^{L(k)} |\psi_k(x)|^2 dx \quad (2)$$

$$\tau_i(k) \equiv -\frac{\hbar}{k} \Im[r(k)] \left(\frac{dk}{dE} \right) \quad (3)$$

$$\tau_g(k) \equiv \tau_d(k) + \tau_i(k) \quad (4)$$

where $\psi_k(x < 0) = e^{ikx} + r(k)e^{-ikx}$ and $\psi_k(x > L) = t(k)e^{ikx}$, $\Im[r(k)]$ is the imaginary part of $r(k)$, $L(k)$ is the separation between where the wave function enters and emerges from a general barrier, $dk/dE = m/\hbar^2 k$, and $\hbar k$ is the momentum of the eigenstate. The transmission and reflection coefficients, $t(k)$ and $r(k)$, respectively, for $V_{rec}(x)$ for $k > k_v$ are [29, 33]

$$\begin{aligned} t_{rec}(k) &= \frac{2k\kappa e^{-ikL}}{2k\kappa \cos(L\kappa) - i(k^2 + \kappa^2) \sin(L\kappa)} \\ r_{rec}(k) &= \frac{-i(k^2 - \kappa^2) \sin(L\kappa)}{2k\kappa \cos(L\kappa) - i(k^2 + \kappa^2) \sin(L\kappa)} \end{aligned} \quad (5)$$

where $\kappa(k) \equiv |k_v^2 - k^2|^{1/2}$ so that κ is chosen to *always* be real and positive. The transmission probability is then

$D_{rec}(k) = |t_{rec}(k)|^2$; for over the barrier,

$$D_{rec}(k > k_v) = \left\{ 1 + \left[\frac{1}{2} \left(\frac{k}{\kappa} - \frac{\kappa}{k} \right) \sin(L\kappa) \right]^2 \right\}^{-1} \quad (6)$$

For $k < k_v$ then $\kappa \rightarrow i\kappa$, causing the trigonometric terms to become their hyperbolic counterparts.

Proceeding with the first step, the Gamow factor for $V_{rec}(x)$ is given by $\theta(k) \equiv 2\sigma\kappa(k)L$, where the tunneling width L is constant and the shape factor $\sigma = 1$ [34, 35]. Invoking half-angle formulae to convert $\cosh(\theta/2)$ and $\sinh(\theta/2)$ to easier forms, then for $k < k_v$

$$\Im[r(k)] = -\frac{2k\kappa k_v^2 \sinh \theta}{k_v^4 [\cosh \theta - 1] + 2(2k\kappa)^2} \quad (7)$$

and therefore

$$\frac{\tau_i(k)}{\tau_o} = \left(\frac{\kappa k_v^4}{k} \right) \frac{\sinh \theta}{k_v^4 (\cosh \theta - 1) + 2(2k\kappa)^2} \quad (8)$$

where $\tau_o = \hbar/V_o$. $\tau_d(k)$ requires the coefficients of the wave function inside the barrier, where $\psi_k(x) = a(k)e^{-\kappa x} + b(k)e^{\kappa x}$. They are solutions to [29, 33, 36, 37]

$$\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \frac{1}{2\kappa} \begin{bmatrix} \kappa - ik & \kappa + ik \\ \kappa + ik & \kappa - ik \end{bmatrix} \begin{pmatrix} 1 \\ r(k) \end{pmatrix} \quad (9)$$

Insertion of $\psi_k(0 < x < L)$ into Eq. (2) and using $\int_0^L e^{\pm 2\kappa x} dx = \pm(L/2)(e^{\pm \theta} - 1)/\theta$ results in

$$\frac{\tau_d(k)}{\tau_o} = \left(\frac{k k_v^2}{\kappa} \right) \frac{k_v^2 \sinh \theta - (k^2 - \kappa^2) \theta}{k_v^4 (\cosh \theta - 1) + 2(2k\kappa)^2} \quad (10)$$

Although the McColl-Hartman effect is conventionally taken as a wide barrier ($L \rightarrow \infty$) limit, here, it is the $\theta \rightarrow \infty$ limit because θ can be large even when κ is small. Therefore, for large θ , τ_d and τ_i are (compare Appendix D, Ref. [18])

$$\tau_d(k) = \tau_o \frac{k}{\kappa} \tanh \theta; \quad \tau_i(k) = \tau_o \frac{\kappa}{k} \tanh \theta \quad (11)$$

so that $\tau_g = \tau_o (k_v^2/k\kappa) \tanh \theta$ is the sum, as per Eq. (4). Hartman’s (and Winful’s) finding that $\tau_g \rightarrow \tau_o k_v^2/k\kappa$ is then recovered when $\theta > 4$ for which $\tanh \theta$ differs from unity by $< 0.07\%$.

However, when $k = k_v$ (or $E = V_o$), the Gamow factor vanishes even though L is finite and large. This entails that as $k \rightarrow k_v$, then the small θ limit is required. Expanding $\sinh \theta$ and $\cosh \theta$ for small θ , replacing $\theta = 2\kappa L$, and then taking the limit $k \rightarrow k_v$ gives

$$\lim_{k \rightarrow k_v} \frac{\tau_d(k)}{\tau_o} = \frac{2Lk_v}{3} \left[\frac{(Lk_v)^2 + 3}{(Lk_v)^2 + 4} \right] \quad (12)$$

$$\lim_{k \rightarrow k_v} \frac{\tau_i(k)}{\tau_o} = \frac{Lk_v}{(Lk_v)^2 + 4} \quad (13)$$

In the large L limit when $k = k_v$, then Hartman's result for τ_g , which would otherwise seemingly diverge as $1/\kappa(k)$, is instead

$$\lim_{L \rightarrow \infty} \frac{\tau_g(k_v)}{\tau_o} = \left(\frac{Lk_v}{3} \right) \frac{2(Lk_v)^2 + 9}{(Lk_v)^2 + 4} \rightarrow \frac{2}{3} Lk_v \quad (14)$$

as per Eq. (4) and therefore *is not independent of the barrier width L* when $k = k_v$. Thus, the independence of barrier width is a large θ limit rather than a large L limit, an important distinction because θ vanishes for $k = k_v$, where $\tau_g(k_v) = \tau_d(k_v)$ are finite. The behavior of τ_d , τ_i , and τ_g are shown in Figures 1 and 2 for increasing L .

Proceeding with the second step, the model of a rectangular barrier is undesirable in the consideration of field emission from a metal because, first (and practically), the tunneling process requires a large electric field to initiate the tunneling and cause it to dominate thermionic emission for which a rectangular barrier model is inadequate, and second (and aesthetically), when $k > k_v$ then the Airy function solutions to Schrödinger's equation behave such that $D_{fn}(k > k_v) \rightarrow 4k\kappa/(\kappa + k)^2$ when the applied field $\mathcal{E} \rightarrow 0$. The triangular barrier is given by

$$V(x > 0) = V_o - Fx \equiv \frac{\hbar^2}{2m} [k_v^2 - fx] \quad (15)$$

and zero for $x < 0$, where $F = q|\mathcal{E}|$ contains the electric field $\mathcal{E}$, and q is the (positive) elementary charge unit, so that the charge of an electron is $-q$. The tunneling length factor L is now dependent upon F in Eq. (15) [38], and therefore

$$L(k) = \frac{V_o - E}{F} = \frac{k_v^2 - k^2}{f} = \frac{\kappa(k)^2}{f} \quad (16)$$

for field emission conditions. For $x > 0$, $\psi_k(x) = t(k) [\text{Ai}(w) - i \text{Bi}(w)]$, where

$$w(x) = \frac{k_v^2 - k^2 - fx}{f^{2/3}} \quad (17)$$

Using the asymptotic forms of the Airy functions, the transmission and reflection factors associated with the barrier of Eq. (15) lead to the self-interference time

$$\frac{\tau_i(k)}{\tau_o} = \frac{\pi f^{1/3} k_v^2 \chi(\theta)}{k [\pi k^2 \Sigma(\theta) + \pi f^{2/3} \Sigma'(\theta) + 2f^{1/3} k]} \quad (18)$$

where for $k < k_v$, $\theta(k) = 4\kappa^3/3f = 2\sigma\kappa L$ for $\sigma = 2/3$ and $L(k) = \kappa^2/f$ [35], and

$$\begin{aligned} \Sigma(\theta) &= \text{Ai}[w(0)]^2 + \text{Bi}[w(0)]^2 \\ \Sigma'(\theta) &= \text{Ai}'[w(0)]^2 + \text{Bi}'[w(0)]^2 \\ \chi(\theta) &= \text{Ai}[w(0)] \text{Ai}'[w(0)] + \text{Bi}[w(0)] \text{Bi}'[w(0)] \end{aligned} \quad (19)$$

FIG. 1. Comparisons of rectangular barrier dwell time τ_d (Eq. (8)), self-interference delay τ_i (Eq. (10)), and group delay τ_g as per Eq. (4) (solid lines) to the asymptotic large- θ form (Eq. (11), dashed lines) for increasing L (top to bottom). Additionally, τ_d in particular is marked with a dot ($\bullet$) symbol, and the green line for τ_g is thin.

The large and small θ -limits have separate behavior. In the large θ limit, $\tau_i(k)$ becomes

$$\frac{\tau_i(k)}{\tau_o} \approx \frac{\kappa k_v^2}{k (k_v^2 + 2k\kappa e^{-\theta})} \quad (20)$$

and therefore approaches $\tau_i(k)/\tau_o \rightarrow \kappa/k$ as $\theta \rightarrow \infty$. In

FIG. 2. The rectangular barrier dwell times $\tau_d(k)$ (Eq. (10)) for various barrier widths L and heights V_o : larger values are associated with larger θ .

the $(k \rightarrow k_v)$ limit where $\theta \rightarrow 0$, $\tau_i(k)$ becomes

$$\begin{aligned} \frac{\tau_i(k_v)}{\tau_o} &= \frac{\pi f^{1/3} k_v \chi(0)}{\pi k_v^2 \Sigma(0) + \pi f^{2/3} \Sigma'(0) + 2f^{1/3} k_v} \\ &= \frac{\sqrt{3}\epsilon}{4\epsilon^2 + 6\epsilon + 3} \end{aligned} \quad (21)$$

where $\epsilon = f^{1/3}/\eta k_v$ where $\eta \equiv (4\pi/3) \text{Bi}(0)^2 = 1.5839$. For finite F , $\tau_i(k_v)$ does not vanish. The behavior of $\tau_i(k)$ therefore mimics its analog for the rectangular barrier, where $f^{1/3}/\eta\sqrt{3}$ takes over the role of $1/L$.

The dwell time $\tau_d(k)$ makes use of

$$\begin{aligned} |\psi_k(x)|^2 &= |t(k)|^2 \Sigma \left(\frac{4}{3} w(x)^{3/2} \right) \\ |t(k)|^2 &= \frac{4\pi k^2}{\pi k^2 \Sigma(\theta) + \pi f^{2/3} \Sigma'(\theta) + 2k f^{1/3}} \end{aligned} \quad (22)$$

where $\theta \equiv 4\kappa^3/3f$ as before, from which

$$\frac{\tau_d(k)}{\tau_o} = |t(k)|^2 \frac{k_v^2}{2k f^{1/3}} \int_0^\theta \frac{\Sigma(u)}{u^{1/3}} du \quad (23)$$

Again, the large and small θ -limits of $\tau_d(k)$ have separate behavior. In the large θ limit

$$\frac{\tau_d(k)}{\tau_o} \approx \frac{5k_v^2 \kappa}{4\pi k f^{2/3}} |t(k)|^2 [1 + \delta(\theta)] \quad (24)$$

$$\delta(\theta) \equiv \frac{1}{15\theta^{1/3}} \int_0^\theta \frac{e^{-z} + 4e^z - 5}{z^{2/3}} dz \quad (25)$$

For large θ , $\delta \approx 4e^\theta/15\theta$ and $|t|^2 \approx 4\pi k^2 \kappa e^{-\theta}/f^{1/3} k_v^2$, so

$$\frac{\tau_d(k)}{\tau_o} \approx \frac{k_v^2 f^{1/3}}{4\pi k \kappa^2} |t(k)|^2 e^\theta = \frac{k}{\kappa} \quad (26)$$

FIG. 3. Comparison of the exact ($\circ, \square, \diamond$) $\tau_i(k)$ (Eq. (18)) and ($\bullet, \blacksquare, \blacklozenge$) $\tau_d(k)$ (Eq. (23)) to the approximations (lines) of Eq. (20) and Eq. (24), respectively. Legend is labeled by values of F [0.1 eV/nm]. $V_o = 1.25$ eV and $\tau_o = 0.52657$ fs. The subscript “ x ” on the τ_x axis label denotes either d or i . τ_g (not shown) would be the sum as per Eq. (4).

with the next order term going as $e^{-\theta}$, akin to Eq. (11). The large θ limit of τ_g is then the sum of Eqs. (21) and (24), as per Eq. (4). In the small θ limit, the integrand in Eq. (23) may use a polynomial expansion for small argument of $\Sigma(u)$ from Eq. (19) and then integrated analytically term by term. It is found

$$\frac{\tau_d(k_v)}{\tau_o} \rightarrow |t(k_v)|^2 \left(\frac{\eta(k_v \kappa)^2}{2\pi f} \right) \left[1 + \frac{\kappa^2}{\sqrt{3}\eta f^{2/3}} \right] \quad (27)$$

which vanishes as κ^2 as $k \rightarrow k_v$ (compare Eq. (12)). The behavior of $\tau_d(k)$ is therefore *in contrast to the behavior of its analog* for the rectangular barrier, where $\tau_d(k)$ remains finite as $k \rightarrow k_v$ for finite L . An evaluation of $\tau_i(k)$ and $\tau_d(k)$ is shown for several representative fields and barrier heights in Figure 3 where, again, τ_g would be found as per Eq. (4). The larger $\theta(E) \propto (V_o - E)^{3/2}/F$ is, the better the approximations are. Notably, if applied to a wave packet composed of many components, and when either L or $1/f$ is large, then the more energetic components will increasingly constitute the outgoing packet, and they will therefore be associated with the smallest $\theta(k)$ factors. Efforts to bypass such complications by making very wide wave packets with a very narrow momentum spreads entail complications for the simulation of tunneling that are difficult. The relation $\tau_d(k)$ and $\tau_i(k)$ to the WDF analysis of wave packets of our prior work shall be taken up separately.

In summary, the behavior of the self-interference τ_i and dwell τ_d times that make up the group delay as per Winful [16, 17] have been reevaluated for the rectangular (or MIM) barrier and extended to the trian-

gular (or field emission) barrier. For the rectangular barrier, the oft made claim that the delay time becomes sensibly independent of the width L of the barrier (the McColl-Hartman effect) applies *only* to conditions where the Gamow factor $\theta(k)$ is large (*e.g.*, where $k < \sqrt{k_v^2 - (2/L)^2}$): when θ is small, then the dwell and self-interference times are in fact dependent on L and in particular $\tau_d(k_v)$ grows with L . For the triangular barrier characterized by the field term F , it was shown that τ_d vanishes as κ^2 , behavior in contrast to the rectangular barrier results. Insofar as the behavior of $\tau_i(k)$ and $\tau_d(k)$ mimic Eq. (11), as remains to be demonstrated, then the shape factor method readily gives the behaviors of their respective Gamow factors $\theta(E)$.

The data that supports the findings of this study are available within the article.

KLJ and AS gratefully acknowledge support from the NRL *Naval Innovative Science and Engineering* (NISE) program. DAS and JR gratefully acknowledge support by the Air Force Office of Scientific Research (AFOSR) through the lab task 18RDCOR016, *Cathode Materials Research for High Power Microwave Sources* and the Air Force Office of Scientific Research *Chief Scientist Laboratory Research Initiative Request #99DE01COR*. JLL was supported by AFOSR under the Award number FA9500-16-10037. RS gratefully acknowledges support from the AFRL *Directed Energy Chief Scientist Office* and the EOARD, grant FA8655-20-1-7002.

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